

Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 03:25 PM EDT

PDB ID	:	2MW2
BMRB ID	:	25296
Title	:	Hha-H-NS46 charge zipper complex
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Deposited on	:	2014-10-24

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

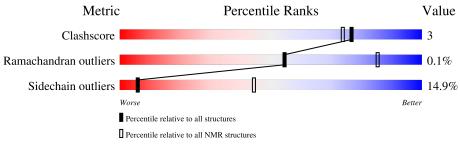
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment is 10%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f NMR} \ { m archive} \ (\#{ m Entries})$
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain		
1	А	72	79%	14%	7%
2	В	47	81%	13%	6%
2	С	47	79%	11%	• 6%



2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues						
Well-defined core Residue range (total) Backbone RMSD (Å) Medoid model						
1	A:6-A:72, B:3-B:46, C:3-	0.80	1			
C:44 (153)						

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 6, 7, 8, 10
2	3, 9
Single-model clusters	4; 5



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2601 atoms, of which 1317 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Hemolysin expression-modulating protein Hha.

Mol	Chain	Residues			Atom	IS			Trace
1	٨	67	Total	С	Η	Ν	0	S	0
	A	07	1145	360	579	98	105	3	0

• Molecule 2 is a protein called DNA-binding protein H-NS.

Mol	Chain	Residues	Atoms				Trace		
2	р	4.4	Total	С	Η	Ν	0	S	0
	D	44	728	218	369	65	74	2	0
2	С	4.4	Total	С	Η	Ν	Ο	S	0
	U	44	728	218	369	65	74	2	0

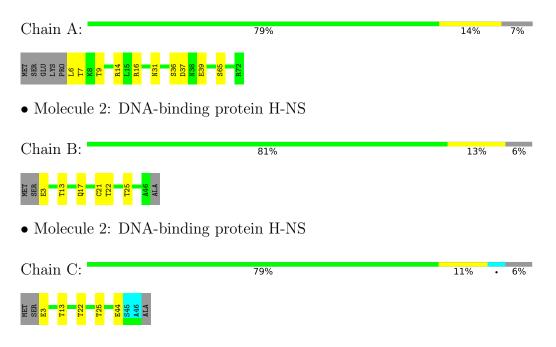


4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

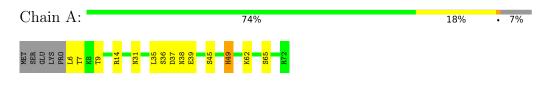
• Molecule 1: Hemolysin expression-modulating protein Hha



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)





• Molecule 2: DNA-binding protein H-NS Chain B: 77% 15% • 6% E E • Molecule 2: DNA-binding protein H-NS Chain C: 66% 23% 6% 4.2.2Score per residue for model 2 • Molecule 1: Hemolysin expression-modulating protein Hha Chain A: 72% 18% 7% . MET SER GLU LYS PRO • Molecule 2: DNA-binding protein H-NS Chain B: 70% 19% 6% MET • Molecule 2: DNA-binding protein H-NS Chain C: 72% 6% 17% 4.2.3Score per residue for model 3 • Molecule 1: Hemolysin expression-modulating protein Hha Chain A: 75% 18% 7% MET SER GLU LYS PRO • Molecule 2: DNA-binding protein H-NS

Chain B:



17%

6%

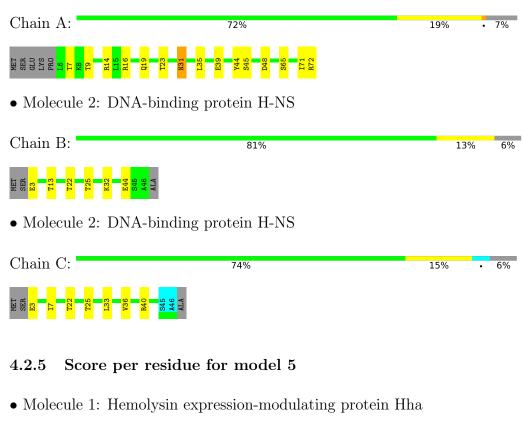
77%

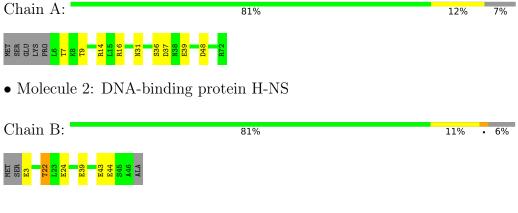


• Molecule 2: DNA-binding protein H-NS



4.2.4 Score per residue for model 4



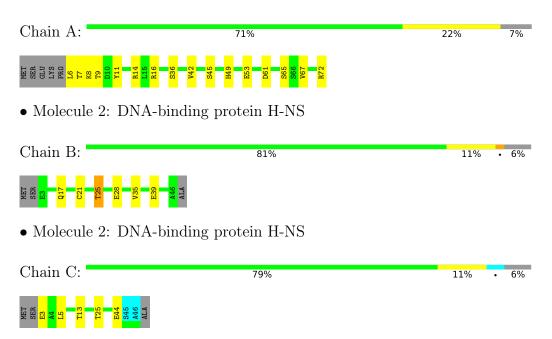


• Molecule 2: DNA-binding protein H-NS



4.2.6 Score per residue for model 6

• Molecule 1: Hemolysin expression-modulating protein Hha

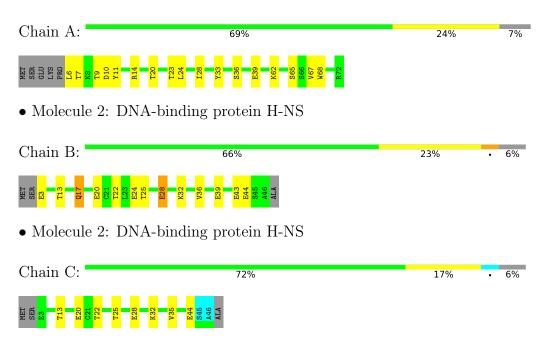


4.2.7 Score per residue for model 7

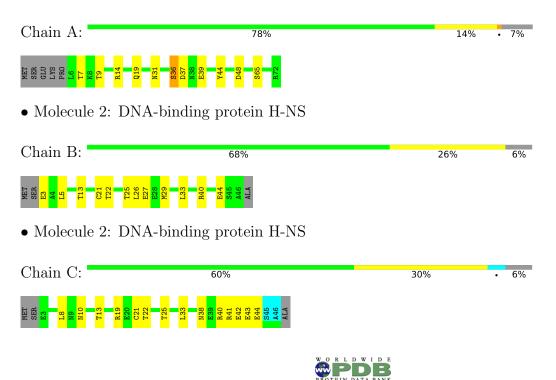
Chain A:	75%	1	.8%	7%
MET SER GLU CYS PRO FRO K8 T3 T3	D10 Y11 Y11 L15 L16 R14 R16 R16 B37 B36 B37 B37			
• Molecule 2	2: DNA-binding protein H-NS			
Chain B:	74%	17	%	• 6%
MET SER E3 E3 L8 L8 L1 L14 R15 R15	C21 T22 E24 T25 E27 A16 A16 A1A			
• Molecule 2	2: DNA-binding protein H-NS			
Chain C:	64%	23%	•	• 6%

4.2.8 Score per residue for model 8

• Molecule 1: Hemolysin expression-modulating protein Hha



4.2.9 Score per residue for model 9



4.2.10 Score per residue for model 10

Chain A:	65%	26%	• 7%
MET SER GLU GLU CVC CVC CVC T7 T7 T7 T7 T7 T7 T7 T7 T7 T7 T7 T7 T7	N31 N31 N33 N336 N337 N338 E339 F43 F43 F43 F43 F43 F43 F43 F43 F43 F43		
• Molecule 2: DNA-	binding protein H-NS		
Chain B:	72%	21%	6%
MET SER SER 111 112 113 114 115 114 115 114 115 114 115 115 115	122 126 M29 A46 ALA		
• Molecule 2: DNA-	binding protein H-NS		
Chain C:	72%	17%	• 6%
MET SER E3 113 113 113 122 122 133 125 133	8345 845 ALA		



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Rigid-body/torsion angle simulated annealing, Cartesian Molecular dynamics.*

Of the 400 calculated structures, 10 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	refinement	2.1
CNS	refinement	2.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	235
Number of shifts mapped to atoms	227
Number of unparsed shifts	0
Number of shifts with mapping errors	8
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	10%



6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	А	566	579	577	3 ± 1
2	В	359	369	368	4 ± 2
2	С	348	359	358	3 ± 2
All	All	12730	13070	13030	78

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

Models Clash(Å) Distance(Å) Atom-1 Atom-2 Worst Total 2:B:21:CYS:SG 2:B:25:THR:HB $\mathbf{2}$ 3 1.561.402:B:21:CYS:SG 2:B:25:THR:CB 2.32 $\mathbf{2}$ 3 1.182:B:21:CYS:SG 2:B:26:LEU:HD21 9 $\overline{2}$ 0.922.042:B:21:CYS:SG 2:B:26:LEU:CD2 0.742.759 22:B:5:LEU:CD2 2:C:21:CYS:SG 0.702.809 1 2 1:A:68:TRP:HB2 2:C:35:VAL:HG11 0.651.697 1:A:6:LEU:N 1:A:11:TYR:HH 0.611.94 73 2:C:38:ASN:O 2:C:42:GLU:HG3 0.552.019 1 1:A:45:SER:O 1:A:49:HIS:HB2 0.532.031 1 1:A:36:SER:HB2 1:A:38:ASN:OD1 2.04 2 0.521 2:C:35:VAL:O 2:C:39:GLU:HG3 0.522.04 $\mathbf{2}$ 1 2:B:17:GLN:O 3 2:B:20:GLU:HG2 2.068 0.50

All unique clashes are listed below, sorted by their clash magnitude.

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2M	W2

Continued from pre				Mo	dels
Atom-1	Atom-2	$\operatorname{Clash}(\operatorname{\AA})$	Distance(Å)	Worst	Total
1:A:68:TRP:HB2	2:C:35:VAL:HG21	0.50	1.82	2	1
1:A:68:TRP:CZ2	2:C:32:LYS:HE2	0.50	2.42	10	1
2:C:38:ASN:O	2:C:41:ARG:HB2	0.49	2.07	7	1
2:B:5:LEU:HD22	2:C:21:CYS:SG	0.49	2.47	9	1
2:B:39:GLU:O	2:B:43:GLU:HG3	0.49	2.07	8	2
2:C:32:LYS:O	2:C:36:VAL:HG23	0.49	2.07	5	2
2:B:33:LEU:HD23	2:C:33:LEU:HD22	0.49	1.83	9	1
2:C:33:LEU:O	2:C:36:VAL:HG12	0.48	2.09	4	1
2:C:40:ARG:HD2	2:C:43:GLU:OE1	0.48	2.09	1	3
2:B:5:LEU:HD23	2:C:21:CYS:SG	0.48	2.47	9	1
2:B:27:GLU:OE2	2:C:41:ARG:HD3	0.47	2.09	7	2
1:A:31:ASN:O	1:A:35:LEU:HG	0.47	2.09	4	2
2:B:21:CYS:HG	2:B:25:THR:HB	0.47	1.55	2	1
2:B:27:GLU:O	2:B:31:GLU:HG3	0.46	2.11	2	1
2:B:31:GLU:O	2:B:35:VAL:HG13	0.46	2.11	2	1
2:B:32:LYS:O	2:B:35:VAL:HG22	0.46	2.10	2	1
1:A:72:ARG:HA	2:B:15:ARG:NH1	0.46	2.26	10	1
2:B:34:GLU:HG3	2:B:35:VAL:N	0.46	2.25	2	1
2:B:35:VAL:O	2:B:39:GLU:HG3	0.45	2.12	6	1
2:C:32:LYS:O	2:C:35:VAL:HG12	0.45	2.12	5	1
1:A:36:SER:O	1:A:37:ASP:HB2	0.45	2.12	3	6
2:B:22:THR:HB	2:B:24:GLU:OE1	0.45	2.12	5	1
2:B:27:GLU:OE1	2:C:41:ARG:HD3	0.44	2.12	9	1
1:A:49:HIS:O	1:A:53:GLU:HG2	0.44	2.12	6	1
1:A:8:LYS:HD2	1:A:45:SER:CB	0.43	2.44	6	1
2:C:28:GLU:O	2:C:32:LYS:HG2	0.43	2.14	8	1
1:A:72:ARG:HA	2:B:15:ARG:NH2	0.43	2.29	7	1
2:B:10:ASN:OD1	2:B:12:ARG:HB2	0.42	2.14	10	1
1:A:24:LEU:O	1:A:28:ILE:HG12	0.42	2.14	8	1
2:C:39:GLU:O	2:C:43:GLU:HG3	0.42	2.14	1	1
1:A:16:ARG:HA	1:A:50:ARG:NE	0.42	2.29	3	2
2:B:15:ARG:HD3	2:C:39:GLU:OE1	0.42	2.15	7	1
2:C:27:GLU:O	2:C:31:GLU:HG3	0.42	2.15	5	1
2:B:26:LEU:O	2:B:29:MET:HG3	0.42	2.14	9	1
2:C:10:ASN:HB3	2:C:13:THR:OG1	0.41	2.15	7	2
2:B:32:LYS:O	2:B:36:VAL:HG23	0.41	2.16	8	1
2:B:28:GLU:O	2:B:32:LYS:HG3	0.41	2.15	8	1
1:A:6:LEU:HB2	1:A:11:TYR:CZ	0.41	2.51	8	1
2:B:29:MET:SD	2:C:33:LEU:HD21	0.41	2.56	10	1
2:B:21:CYS:SG	2:C:5:LEU:HD13	0.40	2.56	1	1
1:A:24:LEU:O	1:A:27:VAL:HG12	0.40	2.16	2	1

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6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	65/72~(90%)	$61 \pm 1 (94 \pm 2\%)$	$4\pm1~(6\pm2\%)$	0±0 (0±0%)	50	82
2	В	42/47~(89%)	42±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	С	41/47~(87%)	41 ± 0 (99 $\pm1\%$)	0±0 (1±1%)	0±0 (0±0%)	100	100
All	All	1480/1660~(89%)	1439 (97%)	40 (3%)	1 (0%)	54	85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	А	21	ILE	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	63/68~(93%)	53 ± 2 (84 $\pm4\%$)	$10\pm2~(16\pm4\%)$	5 42
2	В	40/42~(95%)	$35 \pm 1 (87 \pm 4\%)$	$5\pm1~(13\pm4\%)$	7 48
2	С	39/42~(93%)	$33 \pm 1 \ (85 \pm 3\%)$	$6\pm1~(15\pm3\%)$	6 44
All	All	1420/1520~(93%)	1208 (85%)	212 (15%)	6 44

All 59 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	7	THR	10
1	А	9	THR	10
1	А	14	ARG	10
2	С	25	THR	10

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Mol	Chain	Res	Type	Models (Total)
1	А	39	GLU	9
1	А	65	SER	9
2	В	3	GLU	9
2	В	25	THR	9
2	С	22	THR	9
2	В	22	THR	8
2	С	13	THR	8
2	В	13	THR	7
2	С	44	GLU	7
2	С	3	GLU	6
1	А	16	ARG	5
1	А	36	SER	5
1	А	48	ASP	5
2	В	44	GLU	5
1	А	44	TYR	4
1	А	31	ASN	4
2	В	8	LEU	3
2	В	17	GLN	3
1	А	61	ASP	3
2	В	28	GLU	3
1	А	67	VAL	3
1	А	6	LEU	2
1	А	62	LYS	2
2	С	7	ILE	2
2	С	19	ARG	2
2	С	20	GLU	2
1	А	45	SER	2
2	С	8	LEU	2
2	С	10	ASN	2
2	С	40	ARG	2
1	А	19	GLN	2
1	А	23	THR	2
1	А	72	ARG	2
1	А	42	VAL	2
2	В	24	GLU	2
1	А	49	HIS	1
1	А	27	VAL	1
1	А	58	LYS	1
2	В	34	GLU	1
2	В	38	ASN	1
2	С	27	GLU	1
1	А	13	MET	1

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Mol	Chain	Res	Type	Models (Total)
2	С	38	ASN	1
1	А	71	ILE	1
2	В	32	LYS	1
2	С	24	GLU	1
2	С	39	GLU	1
2	С	5	LEU	1
1	А	22	ASP	1
1	А	10	ASP	1
1	А	20	THR	1
1	А	33	TYR	1
2	В	40	ARG	1
1	А	38	ASN	1
2	С	36	VAL	1

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6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 10% for the well-defined parts and 10% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: assigned_chem_shift_list_1

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	133
Number of shifts mapped to atoms	129
Number of unparsed shifts	0
Number of shifts with mapping errors	4
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

• No matching atom found in the structure. All 4 occurrences are reported below.

List ID	Chain	Dog	Tuno	Atom		Shift Data	l I
	Chain	nes	Type	Atom	Value	Uncertainty	Ambiguity
1	А	3	GLU	Н	8.417	0.020	1
1	А	3	GLU	N	122.711	0.3	1
1	А	4	LYS	Н	8.099	0.020	1
1	А	4	LYS	N	122.518	0.3	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}C_{\alpha}$	0		None (insufficient data)
$^{13}C_{\beta}$	0		None (insufficient data)
$^{13}C'$	0		None (insufficient data)
¹⁵ N	64	1.03 ± 0.25	Should be applied



7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 6%, i.e. 129 atoms were assigned a chemical shift out of a possible 2259. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	124/763~(16%)	62/305~(20%)	0/306~(0%)	62/152~(41%)
Sidechain	3/1420~(0%)	2/913~(0%)	0/437~(0%)	1/70~(1%)
Aromatic	2/76~(3%)	1/36~(3%)	0/37~(0%)	1/3~(33%)
Overall	129/2259~(6%)	65/1254~(5%)	0/780~(0%)	64/225~(28%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 6%, i.e. 129 atoms were assigned a chemical shift out of a possible 2276. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	124/773~(16%)	62/309~(20%)	0/310~(0%)	62/154~(40%)
Sidechain	3/1427~(0%)	2/918~(0%)	0/439~(0%)	1/70~(1%)
Aromatic	2/76~(3%)	1/36~(3%)	0/37~(0%)	1/3~(33%)
Overall	129/2276~(6%)	65/1263~(5%)	0/786~(0%)	64/227~(28%)

7.1.4 Statistically unusual chemical shifts (i)

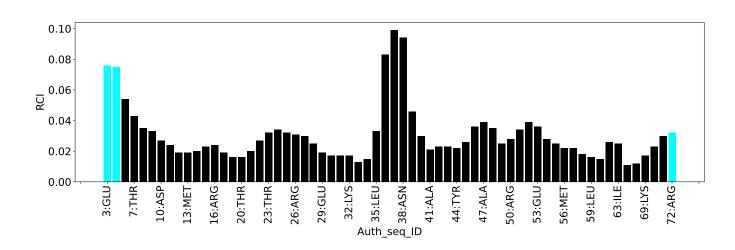
There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:





7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: assigned_chem_shift_list_2

7.2.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	102
Number of shifts mapped to atoms	98
	50
Number of unparsed shifts	0
Number of shifts with mapping errors	4
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

• No matching atom found in the structure. All 4 occurrences are reported below.

List ID	Chain Res	Type Atom		Ros Type			Shift Data	l I
	Chain	nes	Type	Atom	Value	Uncertainty	Ambiguity	
2	В	2	SER	Н	8.203	0.020	6	
2	В	2	SER	N	115.664	0.3	6	
2	В	47	ALA	Н	7.74	0.020	6	
2	В	47	ALA	Ν	128.934	0.3	6	



7.2.2 Chemical shift referencing (i)

Nucleus	# values	${\rm Correction}\pm{\rm precision},ppm$	Suggested action
$^{13}C_{\alpha}$	0		None (insufficient data)
$^{13}C_{\beta}$	0		None (insufficient data)
$^{13}C'$	0		None (insufficient data)
¹⁵ N	45	1.16 ± 0.78	None needed (imprecise)

The following table shows the suggested chemical shift referencing corrections.

7.2.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 4%, i.e. 98 atoms were assigned a chemical shift out of a possible 2259. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	86/763~(11%)	43/305~(14%)	0/306~(0%)	43/152~(28%)
Sidechain	12/1420~(1%)	8/913~(1%)	0/437~(0%)	4/70~(6%)
Aromatic	0/76~(0%)	0/36~(0%)	0/37~(0%)	0/3~(0%)
Overall	98/2259~(4%)	51/1254~(4%)	0/780~(0%)	47/225~(21%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 98 atoms were assigned a chemical shift out of a possible 2276. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	86/773~(11%)	43/309~(14%)	0/310~(0%)	43/154~(28%)
Sidechain	12/1427~(1%)	8/918~(1%)	0/439~(0%)	4/70~(6%)
Aromatic	0/76~(0%)	0/36~(0%)	0/37~(0%)	0/3~(0%)
Overall	98/2276~(4%)	51/1263 (4%)	0/786~(0%)	47/227~(21%)

7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-



defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

